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APPLICATION OF SYMBIOTIC CELLULAR AUTOMATON METHOD TO DESCRIBE THE CONTRAST MEDIA

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Abstract. The method of symbiotic cellular automaton, which combines two approaches to describe the simulated media – the method of conventional cellular automaton and method of movable cellular automaton, has been developed for modeling and study of heterogeneous materials. Verification of the method has been carried out by comparing the simulation results of sorption of carbon dioxide in the lignite with experimental data. Possibilities of the method are exemplified by results of numerical study of the influence of the gas phase on strength and fracture of the lignite specimens.

1 INTRODUCTION

The presence of adsorbed gas in the coal seam produces a significant influence on the mechanical behavior of rock [1 – 3]. At the present time, the adsorbed gas is often considered as the reason of instantaneous outbursts of large quantities of crushed coal, which constitutes a danger to human life and complicates the technological process [4]. So, the early diagnostics of dangerous situation in the seam and prediction of possible hazard is the problem of high importance.

There are many theoretical models, which try to explain the mechanisms of instantaneous outbursts from coal. In general, three factors are considered: stresses, gas and failure of rock [5 – 8]. Despite the fact that the mentioned factors of instantaneous outbursts from coal has been long indicated, we are still far from fully understanding the details of the process. This is due, including the complexity, interconnectivity, dynamics and multiscale processes under consideration, that result in some difficulties in constructing theoretical models. In this context, the methods of computer simulation can be used as effective tool for the theoretical study of the investigated issues. Summarizing the existing theoretical approaches to the analysis of the reasons of instantaneous outbursts of coal, one can note that all approaches consider the mechanical (and sometimes chemical) interaction of gas with a solid frame under high pressure as the fundamental reason of the outbursts. In this regard, in order to adequately investigate the behavior of such media, appropriate methods of description of the behavior of complex multi-phase medium, composed of the coal and mixture of gases (also, in liquefied form) are required.

The modern methods of computer-aided simulation allow the adequate description of the mechanical behavior of media in different states of aggregation. For example, to describe the mechanical behavior of solid medium there is a wide range of methods (finite difference, boundary element, cellular automata [9], et al), of which the most popular is the finite element method, as well as various types of particle method (discrete element, movable cellular automata [10] and other). Simulation of flow of gas and liquid in various porous media and media containing the channels and cracks, is carried out by modern methods such as Lattice Boltzmann [11] and methods based on solving the Navier-Stokes equations on the finite-difference mesh. However, attempts to describe the multiphase medium containing interacting solid, liquid and gaseous phase within a unified approach, met with a number of difficulties arising, in the first place, because of necessity to provide the interconnection between decisions of equations, which are simulating the behavior of each phase. As described in our previous papers [12, 13], successful application of the movable cellular automata (MCA) method on the field of mechanical investigation of the lignite failure, dictated the further development with the incorporation of the conventional cellular automata (CCA) method. Such development originated symbiotic cellular automata (SCA) method that enabled the investigation of the influence of mine gases.

Early the SCA method was verified within the simulation of sorption processes in lignite. The main aim of the present paper is to continue the development and improvement of the suggested approach in order to describe the multiphase system on example of Velenje lignite and to verify the results of modeling with experimental data of coal sample behavior in gas atmosphere under external loading. Although the results of the SCA method in the paper don't represent the final conclusions that would explain the influence of gas as a whole, they still can be used as a good starting-point for the further development of the method and for elaboration of the different mechanical-gas models.

2 DESCRIPTION OF THE METHOD AND MAIN EQUATIONS

Symbiotic cellular automata method is a combination of CCA and MCA approaches [12 - 14]. In the framework of this method the investigated medium is considered as a superposition of two interrelated media. One of them is described by a set of movable cellular automaton and another – by a mesh of conventional cellular automaton. The step of calculation consists of two main substeps. First of them is the step of the MCA model. It is called "mechanical step". At this substep motion equations of movable automata are solved. In other words, the process of mass transfer of solid due to mechanical loading is considered at the first substep. In the framework of the MCA method, we consider the simulated media as an ensemble of interacting finite size elements (automata) [10]. The concept of the MCA method is based on conventional concept of cellular automata developed by means of incorporating of some basic postulates and relations of approach of particle-based methods [13].

The movable cellular automaton is an object of finite size, possessing translational and rotational degrees of freedom. Interaction between automata is defined by normal (acting along the line connecting the mass centers) and tangential forces, each of which is the sum of the corresponding potential and the dissipative component. Within the MCA approach a many-body interaction is used. Furthermore, new types of states, viz., and the state of a pair of

automata in comparison to conventional cellular automaton method are introduced. The new type of state leads to a new parameter which defines the criteria for switching of the inter-automata relationships – the automata overlapping parameter: $h^{ij} = r^{ij} - r_o{}^{ij}$. Here r^{ij} is the initial distance between the centres of the neighbouring elements, and $r_o{}^{ij}$ is defined as $r_o{}^{ij} = (d^i + d^j)/2$, where $d^{i(j)}$ is the automaton size. In the simplest case there are two states of the pair: linked ($h^{ij} < h^{ij}{}_{max}$) and unlinked ($h^{ij} > h^{ij}{}_{max}$). $h^{ij}{}_{max}$ means some critical value defined by investigated problem. The linked state is indicative of chemical bonds between elements and the unlinked state indicates that there is no chemical bond between them.

According to the bistable automata concept (linked – unlinked) the Wiener-Rosenbluth model [15] can be used to define the normal potential force of interaction between *i*-th and *j*-th automata in approximation of nearest neighbours:

$$F_{np}^{ij} = p_{ij} + m_{ij}\left[\sum_{k\neq j} C(ij,ik)\left(\frac{1}{m_i}+\frac{1}{m_k}\right)p_{ik} + \sum_{l\neq i} C(ij,jl)\left(\frac{1}{m_j}+\frac{1}{m_l}\right)p_{jl}\right] \quad (1)$$

Here $p_{ij(ik,jl)}$ is the corresponding pair potential force defined by the automaton response function; $m_{i(j,k,l)}$ is the mass of automaton and $m_{ij} = (m_i m_j / (m_i + m_j))$. The coefficients $C(ij,ik)$ are associated with the rate of perturbation transfer from pair *ik* to pair *ij* and were equal to 1. In the present realization of the MCA model a pair approximation is used to determine the tangential potential force F_{tp}^{ij}. Forces of inter-automata interaction consist of potential and viscous parts, where dissipative forces depend on relative normal and tangential velocities.

Due to automata represents an element of the simulated media the experimental stress-strain curve can be taken as a draft approximation of the response function for inter-automata interaction. In this case the relative overlapping can be considered as deformation in normal direction (ε^{ij}) and specific force (stress) σ^{ij} can be introduced for each automaton as normal force per contact square. In a similar manner it is possible to define shear strain γ^{ij} and stress τ^{ij} of *i* and *j* automata in *i-j* pair. In the simplest case the linear approximation of real complex stress-strain curve can be used to represent the automaton response function in terms of stress (σ) and strain (ε). Depending on the theory and simulated material properties the inter-automata interaction can be represented by response functions of different types. For example, the elastic properties of brittle materials can be described as simple linear response. In this case the loading and unloading will follow the same curve. To take into account the damage generation at a scale level lower than automaton size, the degradation response function should be used. In this case linear response is observed in the range of loading $<0–\sigma_{y1}>$, whereas in the range of $<\sigma_{y1}–\sigma_s>$ damage is generated within automata and the response function is non-linear in character. Furthermore, for the same reason, unloading is defined by a new Young's modulus. The determination of the response function for describing the irreversible behaviour is a challenging problem and requires intimate knowledge of the mechanisms of plastic flow initiation and evolution.

Next for the mechanical – "net" substep is performed on a mesh of conventional cellular automata. At this substep the process of mass transfer of gas in the pores and channels is considered, as well as the values of the forces acting on the movable cellular automata from gas phase are calculated. The configuration of pores and channels through which gas propagates, is projected to the mesh of conventional cellular automata from the MCA layer.

This symbiotic approach combines solutions of mechanical and gas dynamic problems and allows description of multiphase heterogeneous media. It is necessary to note that accuracy of symbiotic automaton method depends on the relation between the size of grid cell and movable automaton diameter. With decreasing this ratio the accuracy of simulation will increase.

The algorithm of projection of movable automata on unmovable mesh takes into account the degree of overlapping of automata and unmovable cell. For example, in the case of superposition of two automata on the cell, the sort of the cell is defined by the sort of movable automaton, which occupies the most part of the cell. The state of this cell is solid. The cell, which is not occupied by any movable automaton, has another state – gaseous or liquid state. This cell is a part of surroundings and can be filled by gas or fluid. In the case of gas it is characterized by temperature T, pressure P and gas (or gases) molar concentration μ. This cell does not take part in the mechanical behavior of the system but it exerts influence on neighboring movable automata by gas pressure.

During simulation of response and fracture of porous solids with gases inside pores it is necessary to estimate volumes of pores and macro-cracks in the specimen. Also, it is necessary to consider the amount of gas, which is dissolved in the bulk of material. For this aim the special parameter of concentration of absorbed gases in the volume of automaton was introduced into the model. In the present model, the Mendeleyev-Clapeyron equation is applied to describe the state of gaseous phase:

$$PV = NR_{gas}T\ , \tag{2}$$

where P is the pressure of gas, N is the number of moles of gas in the volume V, T is current temperature of gas.

There are two types of sorption processes on the boundaries between solid material and closed free volumes and surroundings filled with gases: adsorption of gas on the surface of solid phase and desorption of gas to the volume of pore, crack or surroundings. These two processes are the manifestations of one complex sorption process on the inter-phase boundary.

In a very wide range of gas concentrations in solids and in the surrounding atmosphere it is possible to consider adsorption and desorption processes as independent. In the simplest case these processes are described by the following linear equations:

$$I_{ads} = \alpha_{ads}(\mu_{solid}^{\max} - \mu_{solid})\mu_{env}\ , \tag{3}$$

– intensity of adsorption process ($[I_{ads}] = \frac{mole}{s * m^2}$),

$$I_{des} = K_{des}(\mu_{solid} - \mu_{solid}^{\min})\ , \tag{4}$$

– intensity of desorption process ($[I_{des}] = \frac{mole}{s * m^2}$).

Here α_{ads} – adsorption intensity coefficient; $K_{ads(des)}$ – is the desorption coefficient, μ_{env} – is the concentration of the gas in the atmosphere; μ_{solid} – is the concentration of the gas in solid (material of the specimen); $\mu_{solid}^{\min}$ .and $\mu_{solid}^{\max}$ – are the minimal and maximal possible concentrations of gas in solid, consequently.

Note that both sorption coefficients are not the constants but the functions of material and gas physico-chemical properties. It means that $K_{ads(des)}$ depends on chemical compatibility of molecules of gas and solid. One of the manifestations of this dependence is so-called saturated concentration of gas in the material of the specimen $\mu_{solid}^{\max}$. $K_{ads(des)}$ are also the functions of morphology of the surface of solid. It means that intensity of sorption process strongly depends on microstructure of the surface.

The change of quantity of gas in the closed free volume is calculated as follows:

$$\Delta N_i^{sorp} = S\Delta t \sum_{k=1}^{N_{bound}} \left(I_k^{des} - I_k^{ads} \right), \tag{5}$$

where k – is the number of boundary cells in the volume, Δt – is the time step, N_{bound} – is the number of cells at the boundary with solid. The values of sorption intensities I_{ads} and I_{des} were obtained from the experimental data, proposed in the paper [16].

The presence of gas in the surrounding of solid-state components (or in macropores), as well as in the bulk material (discontinuities in the structure, taken into the accounted implicitly), leads to additional forces acting on the solid surface and causing the growth of internal stresses in the bulk of material. In the simplest approximation it is believed, as that the pressure of surrounding gas to the surface (or part of the surface) of movable automaton is applied normally to it, as this pressure leads only to translation motion of movable automaton.

In addition, the external (from the macropores) and internal (from the "micropores") gas pressure leads to a change in stress state of movable cellular automata. In the framework of the formalism of calculation of the potential interaction of movable cellular automata this effect can be taken into the account by including of the additional pressure into the expression for the medium stress in the pair of movable automata. In the simplest case, when the porosity of the solid material is small, and the characteristic pore sizes are much smaller than the average distance between them, the linear approximation of value of this additional pressure of gas in pores P_{gas}^k can be defined as follows:

$$P_{gas}^k = P_{pores}^k \nu_k, \tag{6}$$

where P_{pores}^k is pore pressure in the volume of a k-th automaton, ν_k – porosity of the material.

3 SIMULATION OF FRACTURE OF DETRITUS IN THE ATMOSPHERE OF CARBON DIOXIDE

As we further investigate the mechanical response in the presence of gases for only pure lithotype varieties, model input data are shown only for fine detrital (dD) and xylite rich (Ks) lignite. Xylite and detritus properties were derived from the characteristic points of the diagram σ – ε and assigned to the single movable cellular automaton. Following the curves on Fig. 1, Y_o is the starting point of the diagram, Y_1 is plastic limit, Y_c point of failure and Y_2 intermediate point which enabled interpolation of non-linear part of the curve. Characteristic points of the diagram on Fig. 1 are actually average values of fine detrital and xylite rich lignite samples, therefore both model curves represent average properties of both chosen lignite varieties.

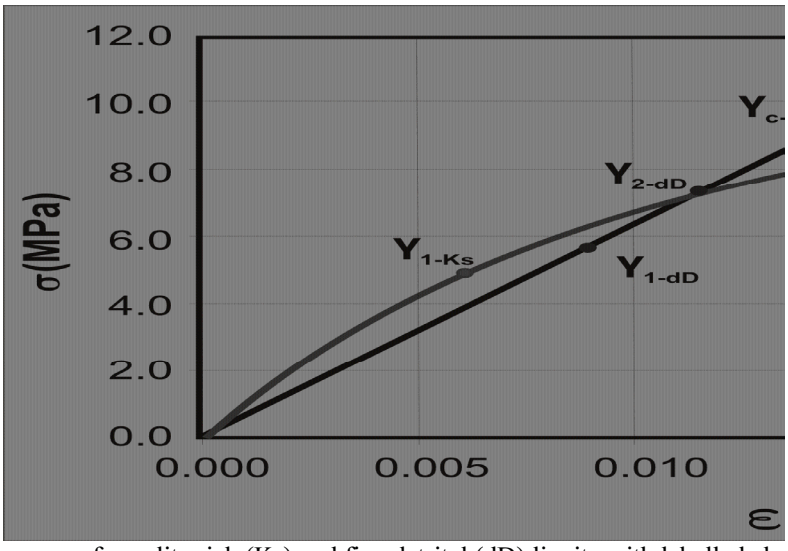

Figure 1: Diagram σ – ε for xylite rich (Ks) and fine detrital (dD) lignite with labelled characteristic points Y_1,Y_2 and Y_c

In addition to defined certain characteristic points *Y*, modeling requires also input of basic mechanical properties of lignite composite such as volume weight (ρ), Young modulus (E), Poisson's ratio (υ), which are shown in Table 1.

Both lignite varieties show due to their mechanical properties very similar strength and elastic properties. Chosen parameters were used for mechanical modeling as an input data for appurtenant movable cellular automata that enable modeling of lignite samples with different lithotype composition.

It is evident from the diagram on Fig. 1 that properties of chosen lignite lithotypes significantly differ. Consequently their response to underground stresses (applied loads) correspond the difference in curve properties. Although the general mechanical properties are rather similar, differences of lignite reflect above all from a shape of stress strain characteristic curves. As the response of the xylite is mostly un-linear and very ductile regarding the structure of the wooden fibres, the curve of the detritus samples is linear and the deformation elastic and recurring.

Table 1: General model mechanical properties of chosen lignite varieties

Properties	Unit	Xylite Ks	Detrite dD
ρ	[kN/m^3]	12,3	12,4
E	[MPa]	743	659
μ	[ ]	0,3	0,3

To demonstrate the possibilities of SCA method and its applicability for describing the "porous solid – gas" media, a series of calculations have been done. In these calculations the

effect of the gas phase (CO_2) on the mechanical response and the failure of the samples of fine detritus were studied. Mechanical properties of fine detritus and xylite inclusions were used as given in [3]. The response and failure of fine detritus under uniaxial compression of CO_2 in the atmosphere and in vacuum were simulated. Size of specimens was 5x10cm, loading rate was v = 0.02 m/sec. Volume concentration of CO_2 in fine detritus and xylite was set equal to the characteristic values in coal seams under the lateral pressure from 1 to 42 bar. In this way the loading of with gas pre-saturated sample of lignite, extracted from the coal seam and tested in laboratory conditions, was simulated.

Fig. 2 shows the results of simulation, reflecting the evolution of the structure of inter-automata links for considered cases a, b, and c. These cases are: a) uniaxial compression of fine detrite specimen (P_{gas} = 0 bar), b) compression of fine detrite specimen using contrained conditions of CO_2 at the pressure of 1 bar without allowing sorption and c) compression of fine detrite specimen in the atmosphere of CO_2 at the pressure of 1 bar and allowing the sorption processes. Typically, the behavior of the simulated samples at initial stage of loading is identical. Place of birth of fractures is an area of the interface between the xylite inclusions and fine detritus matrix.

According to Fig. 2 a,b,c, failures occur at approximately the same values of strain ~1.20%. However, if in the absence of gaseous atmosphere, the crack appears when the strain is 1.23%, then in the presence of the gas atmosphere (contrained gas pressure) the crack is formed within the deformation of 1.25%. Furthermore, differences of evolution only increase. Approximately identical pictures with cracks can be identified with the deformations of 1.28% in the absence of gas atmosphere and of 1.33% in the presence of an atmosphere of CO_2.

Complete destruction of the sample in vacuum occurs by means of the formation of a crosscutting diagonal macro-crack. This corresponds to a deformation of ~1.35%. The destruction of the sample in Fig. 2b occurs by the formation of vertical cracks, which occur at the deformation of 1.45%. Also, many inter-automata links are broken in the upper part of the sample.

The increase of surrounding atmosphere pressure from 0 to 1 bar resulted in an increase of strength and ultimate strain of specimens at 2–5% without a noticeable change in Young's modulus. Also, the fracture pattern of specimens has undergone some changes. The results suggest that even relatively low atmospheric pressure of CO_2 gas is able to exert some influence on the response and the fracture of materials having relatively low strength. As shown in Fig. 2c, accounting of sorption processes during simulation leads to the increase of the number of small damages in the specimen on the final stages of fracture (crushing of material caused by the gas CO_2). However, as shown by simulation at low level of gas pressure, the strength of the sample in these conditions does not change, regardless of the accounting sorption processes in the model.

Obtained results are in agreement with the thesis of [7]: condensed gas in the coal is considered as the reason of instantaneous outburst of crushed coal. The shock wave during the crack propagation initiates phase transformation of condensed gas into gaseous state that provokes the outburst. So, the role of gas in breaking the coal into pieces after the mechanical failure of lignite is significant. The next step of our research is to continue the study of the phenomenon using much higher gas pressure in order to investigate the consequences of very large pressure gradients over short distance and time.

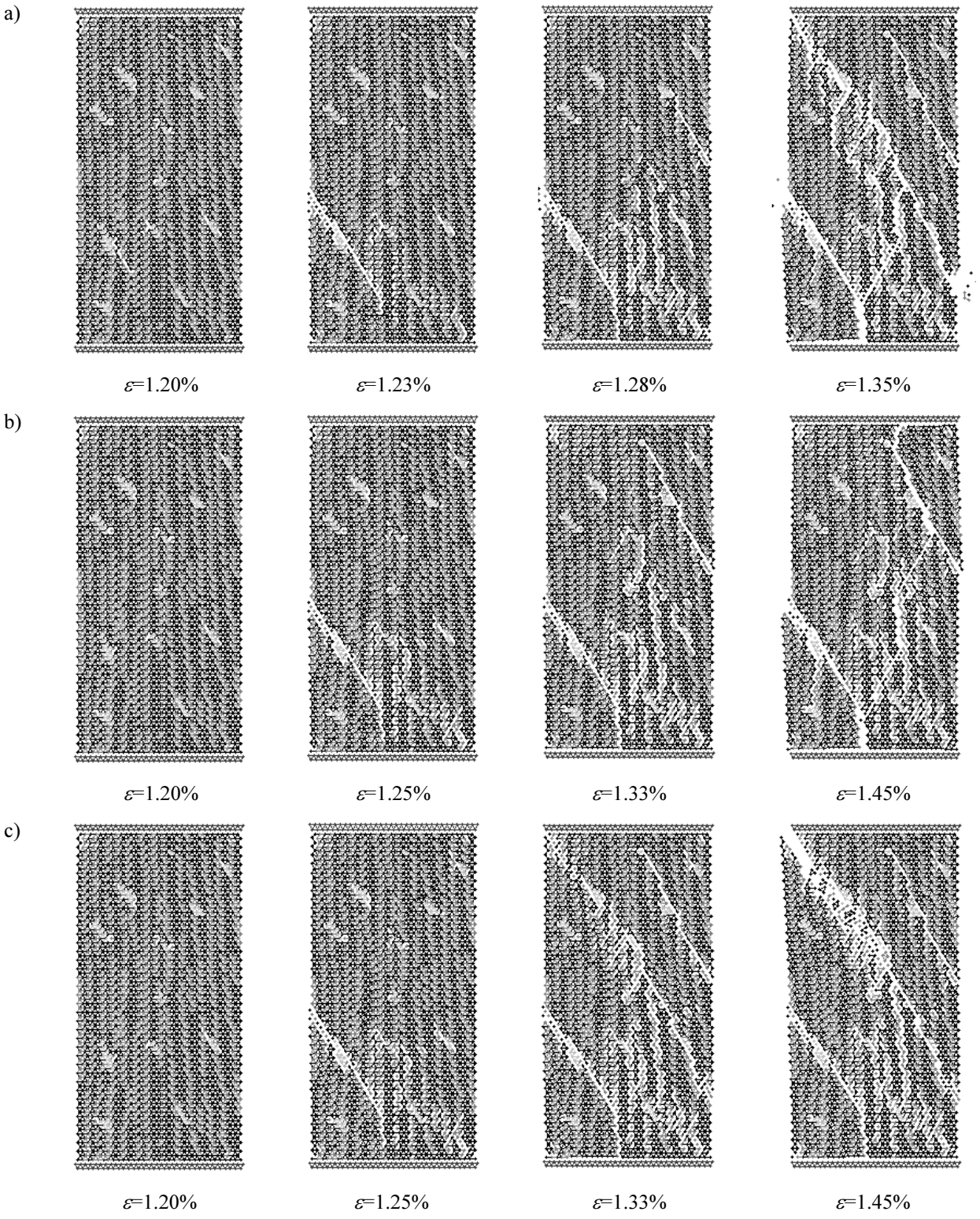

Figure 2: Stages of the fracture of model specimen of fine detritus in the atmosphere of CO_2: a) P_{gas} = 0 bar, without sorption; b) P_{gas} =1 bar, without sorption; c) P_{gas} =1 bar, with sorption

4 CONCLUSIONS

The approach, describing the behavior of two-phase medium under external influence, is proposed. This approach, called as SCA method, represents the combination of methods of conventional and movable cellular automata. Verification of this approach was carried out by means of comparison of the results of modeling of the fine detritus specimens in the CO_2 atmosphere with the results of experimental studies described in [3]. The results demonstrate a qualitative agreement between model and experimental data. It is proposed to use the SCA method to describe the mechanical response of coals with explicit taking into the account the influence of high-pressure gas atmosphere, as well as sorption processes.

It is clear that the proposed approach does not cover the entire spectrum of processes in such a complex system like a multiphase heterogeneous medium. In particular, the proposed model does not take into account the filtration processes, the phase transitions etc. In addition, since the simulated physical processes have different (several orders of magnitude) characteristic times, within the framework of the proposed approach it is possible to simulate adequate only the first few seconds of outburst phenomena. Furthermore, we use a 2D approximation of the simulated object. Of course, these restrictions greatly influence the outcome of the investigated problem.

Nevertheless, proper selection of model parameters allows obtaining good agreement with the results of natural experiments. This demonstrates the correct formulation of the problem and qualitatively correct description of the basic processes occurring in the system.

Further directions of development of the method are the introduction to the model the state equation for non-ideal gas, which is important for realistic CO_2 simulation, as well as the possibility of modeling filtration processes in porous solid body.

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